

10/522, 622 12/15/2006

KOH $\text{II} \rightarrow \text{I}$

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 12:29:37 ON 15 DEC 2006

=> file casreact
COST IN U.S. DOLLARS
SINCE FILE
ENTRY
TOTAL
SESSION
0.21
0.21
FULL ESTIMATED COST

FILE 'CASREACT' ENTERED AT 12:29:52 ON 15 DEC 2006
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FILE CONTENT:1840 - 11 Dec 2006 VOL 145 ISS 24

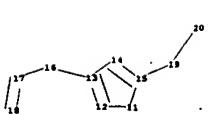
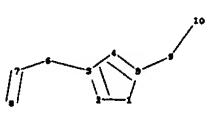
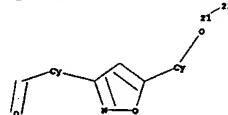
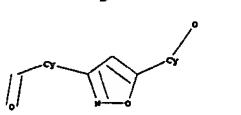
New CAS Information Use Policies, enter HELP USAGETERMS for details.

*
* CASREACT now has more than 10 million reactions
*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>
Uploading C:\Program Files\Stnexp\Queries\10522622\1.KOH+II-I.str



```

chain nodes :
 6 7 8 9 10 16 17 18 19 20 21 22
ring nodes :
 1 2 3 4 5 11 12 13 14 15
chain bonds :
 3-6 5-9 6-7 7-8 9-10 13-16 15-19 16
ring bonds :

```

10/522, 622 12/15/2006

10/522, 622 12/15/2006

1-2 1-5 2-3 3-4 4-5 11-12 11-15 12-13 13-14 14-15
exact/norm bonds :
1-2 1-5 2-3 3-4 3-6 4-5 5-9 6-7 7-8 9-10 11-12 11-15 12-13 13-14 13-16
14-15 15-19 16-17 17-18 19-20
exact bonds :
21-22

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:CLASS
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:Atom
20:CLASS 21:CLASS 22:CLASS
fragments assigned product role:
containing 11
fragments assigned reactant/reagent role:
containing 1
containing 21

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s 11 full
FULL SEARCH INITIATED 12:30:13 FILE 'CASREACT'
SCREENING COMPLETE - 6077 REACTIONS TO VERIFY FROM 455 DOCUMENTS
100.0% DONE 6077 VERIFIED 3 HIT RXNS 2 DOCS
SEARCH TIME: 00.00.02

L2 2 SEA SSS FUL L1 (3 REACTIONS)

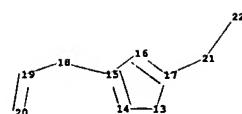
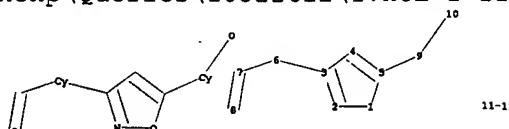
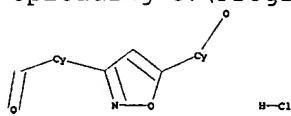
=> d ibib hit 1-2

10/522, 622 12/15/2006

10/522, 622 12/15/2006

I HCl → III

=>
Uploading C:\Program Files\Stnexp\Queries\10522622\1.HCL+I-III.str



chain nodes :

6 7 8 9 10 11 12 18 19 20 21 22

ring nodes :

1 2 3 4 5 13 14 15 16 17

chain bonds :

3-6 5-9 6-7 7-8 9-10 11-12 15-18 17-21 18-19 19-20 21-22

ring bonds :

1-2 1-5 2-3 3-4 4-5 13-14 13-17 14-15 15-16 16-17

exact/norm bonds :

1-2 1-5 2-3 3-4 3-6 4-5 5-9 6-7 7-8 9-10 13-14 13-17 14-15 15-16 15-18

16-17 17-21 18-19 19-20 21-22

exact bonds :

11-12

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:CLASS

11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS

20:CLASS 21:Atom 22:CLASS

fragments assigned product role:

containing 13

fragments assigned reactant/reagent role:

containing 1

containing 11

L3 STRUCTURE UPLOADED

=> d

L3 HAS NO ANSWERS

L3 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s 13 full

FULL SEARCH INITIATED 12:31:00 FILE 'CASREACT'

SCREENING COMPLETE - 23962 REACTIONS TO VERIFY FROM 1991 DOCUMENTS

100.0% DONE 23962 VERIFIED 5 HIT RXNS
SEARCH TIME: 00.00.04

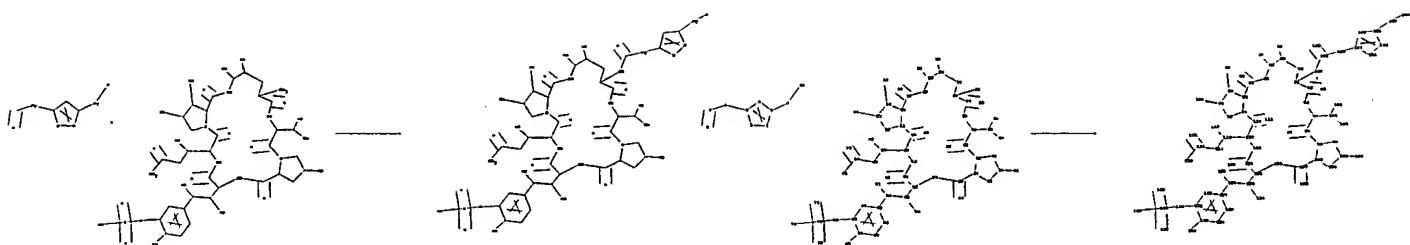
2 DOCS

L4 2 SEA SSS FUL L3 (5 REACTIONS)

=> d ibib hit 1-2

10/522, 622 12/15/2006

(III)(IV) → (V)



chain nodes :

6	7	8	9	10	16	18	21	22	26	28	32	38	39	40	41	43	44	46	48	49	50	51
52	55	58	59	60	61	68	69	70	71	72	73	74	82	84	87	88	93	97	103	104	105	
106	108	109	111	113	114	115	116	117	120	123	124	125	126	133	134	135	136					
137	138	139	140	141	142	143	149	150														

ring nodes :

1	2	3	4	5	11	12	13	14	15	17	19	20	23	24	25	27	29	30	31	33	34	35	36
37	42	45	47	53	54	56	57	62	63	64	65	66	67	77	78	79	80	81	83	85	86		
89	90	91	92	94	95	96	98	99	100	101	102	107	110	112	118	119	121	122	127				
128	129	130	131	132	144	145	146	147	148														

chain bonds :

3-6	5-9	6-7	7-8	9-10	13-44	14-16	17-18	20-21	22-23	25-26	27-28	30-38	31-32									
35-41	38-39	38-40	42-43	45-46	47-48	48-49	48-52	49-50	50-51	50-73	54-55	56-58										
58-59	58-60	60-61	60-62	65-68	66-69	69-70	70-71	70-72	70-74	79-109	80-82											
83-84	86-87	88-89	91-140	92-93	95-103	96-97	100-106	103-104	103-105	107-108												
110-111	112-113	113-114	113-117	114-115	115-116	115-138	119-120	121-123	123-124													
123-125	125-126	125-127	130-133	131-134	134-135	135-136	135-137	135-139	140-141													
141-142	141-143	143-147	145-149	149-150																		

ring bonds :

1-2	1-5	2-3	3-4	4-5	11-12	11-15	11-45	12-13	13-14	14-15	15-17	17-19	19-20									
20-23	23-24	24-25	25-27	27-29	29-30	30-31	31-33	33-34	33-37	34-35	35-36	36-37										
37-42	42-57	45-47	47-53	53-54	54-56	56-57	62-63	62-67	63-64	64-65	65-66											
66-67	77-78	77-81	77-110	78-79	79-80	80-81	81-83	83-85	85-86	86-89	89-90											
90-91	91-92	92-94	94-95	95-96	96-98	98-99	98-102	99-100	100-101	101-102												
102-107	107-122	110-112	112-118	118-119	119-121	121-122	127-128	127-132	128-129													
129-130	130-131	131-132	144-148	144-145	145-146	146-147	147-148															

exact/norm bonds :

1-2	1-5	2-3	3-6	4-5	5-9	6-7	7-8	9-10	11-12	11-15	11-45	12-13	13-14										
14-15	14-16	15-17	17-18	17-19	19-20	20-21	20-23	22-23	23-24	24-25	25-26	25-27											
27-28	27-29	29-30	30-31	31-32	31-33	33-34	33-37	34-35	35-36	35-41	36-37												
37-42	38-39	42-43	42-57	45-46	45-47	47-53	48-52	50-51	50-73	53-54	54-55	54-56											
56-57	58-59	60-61	65-68	66-69	69-70	77-78	77-81	77-110	78-79	79-80	80-81												
80-82	81-83	83-84	83-85	85-86	86-87	86-89	88-89	89-90	90-91	91-92	91-140												
92-93	92-94	94-95	95-96	96-97	96-98	98-99	98-102	99-100	100-101	100-102													
101-102	102-107	103-104	107-108	107-122	110-111	110-112	112-118	113-117	115-116														
115-138	118-119	119-120	119-121	121-122	123-124	125-126	130-133	131-134	134-135														
140-141	141-142	141-143	143-147	144-148	144-145	145-146	145-149	146-147	146-148														
149-150																							

exact bonds :

13-44	30-38	38-40	47-48	48-49	49-50	56-58	58-60	60-62	79-109	95-103	103-105												
112-113	113-114	114-115	121-123	123-125	125-127																		

normalized bonds :

62-63	62-67	63-64	64-65	65-66	66-67	70-71	70-72	70-74	127-128	127-132	128-129												
129-130	130-131	131-132	135-136	135-137	135-139																		

10/522,622 12/15/2006

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:CLASS
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:Atom 18:CLASS 19:Atom
20:Atom 21:CLASS 22:CLASS 23:Atom 24:Atom 25:Atom 26:CLASS 27:Atom 28:CLASS
29:Atom 30:Atom 31:Atom 32:CLASS 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom
38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:Atom 43:CLASS 44:CLASS 45:Atom 46:CLASS
47:Atom 48:CLASS 49:CLASS 50:CLASS 51:CLASS 52:CLASS 53:Atom 54:Atom 55:CLASS
56:Atom 57:Atom 58:CLASS 59:CLASS 60:CLASS 61:CLASS 62:Atom 63:Atom 64:Atom
65:Atom 66:Atom 67:Atom 68:CLASS 69:CLASS 70:CLASS 71:CLASS 72:CLASS 73:CLASS
74:CLASS 77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:CLASS 83:Atom 84:CLASS
85:Atom 86:Atom 87:CLASS 88:CLASS 89:Atom 90:Atom 91:Atom 92:Atom 93:CLASS
94:Atom 95:Atom 96:Atom 97:CLASS 98:Atom 99:Atom 100:Atom 101:Atom 102:Atom
103:CLASS 104:CLASS 105:CLASS 106:CLASS 107:Atom 108:CLASS 109:CLASS 110:Atom
111:CLASS 112:Atom 113:CLASS 114:CLASS 115:CLASS 116:CLASS 117:CLASS 118:Atom
119:Atom 120:CLASS 121:Atom 122:Atom 123:CLASS 124:CLASS 125:CLASS 126:CLASS
127:Atom 128:Atom 129:Atom 130:Atom 131:Atom 132:Atom 133:CLASS 134:CLASS
135:CLASS 136:CLASS 137:CLASS 138:CLASS 139:CLASS 140:CLASS 141:CLASS 142:CLASS
143:Atom 144:Atom 145:Atom 146:Atom 147:Atom 148:Atom 149:Atom 150:CLASS

fragments assigned product role:

containing 77

fragments assigned reactant/reagent role:

containing 1

containing 11

L5 STRUCTURE UPLOADED

=> s 15 full
FULL SEARCH INITIATED 12:46:32 FILE 'CASREACT'
SCREENING COMPLETE - 2 REACTIONS TO VERIFY FROM 1 DOCUMENTS

100.0% DONE 2 VERIFIED 2 HIT RXNS 1 DOCS
SEARCH TIME: 00.00.01

L6 1 SEA SSS FUL L5 (2 REACTIONS)

=> d ibib hit 1

10/522,622 12/15/2006

SINCE FILE ENTRY 118.68	TOTAL SESSION 361.01
-------------------------------	----------------------------

FILE 'REGISTRY' ENTERED AT 12:51:24 ON 15 DEC 2006
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 14 DEC 2006 HIGHEST RN 915690-78-7
DICTIONARY FILE UPDATES: 14 DEC 2006 HIGHEST RN 915690-78-7

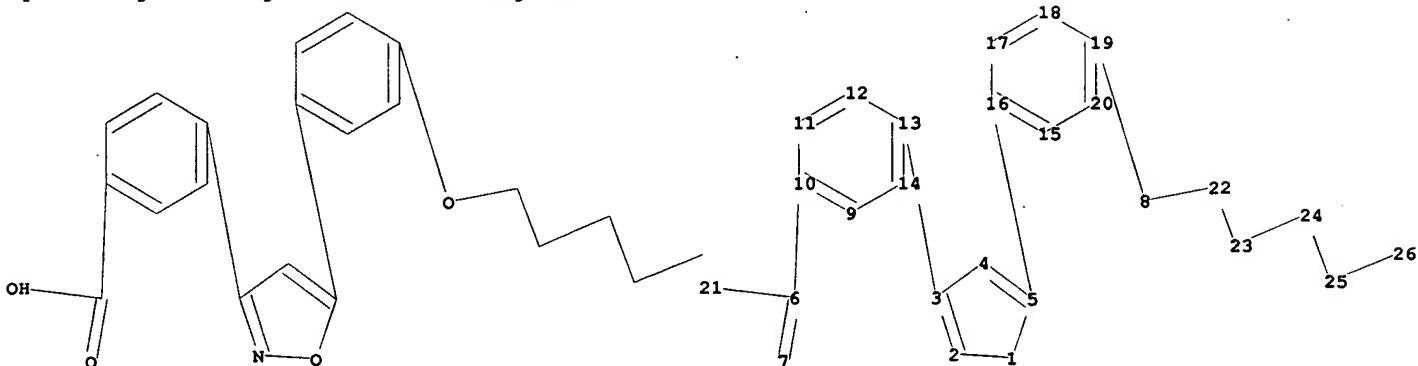
TEGA INFORMATION NOW CURRENT THROUGH June 20, 2006

Please note that search-term pricing does apply when conducting Smart SELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/reqprops.html>

=>
Uploading C:\Program Files\Stnexp\Queries\10522622\17.str



```

chain nodes :
6 7 8 21 22 23 24 25 26
ring nodes :
1 2 3 4 5 9 10 11 12 13 14
chain bonds :
3-13 5-16 6-7 6-10 6-21 8-19
ring bonds :
1-2 1-5 2-3 3-4 4-5 9-10 9-14
17-18 18-19 19-20
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 8-19 8-22

```

10/522, 622 12/15/2006

exact bonds :

3-13 5-16 6-10 22-23 23-24 24-25 25-26

normalized bonds :

6-7 6-21 9-10 9-14 10-11 11-12 12-13 13-14 15-16 15-20 16-17 17-18 18-19
19-20

Match level :

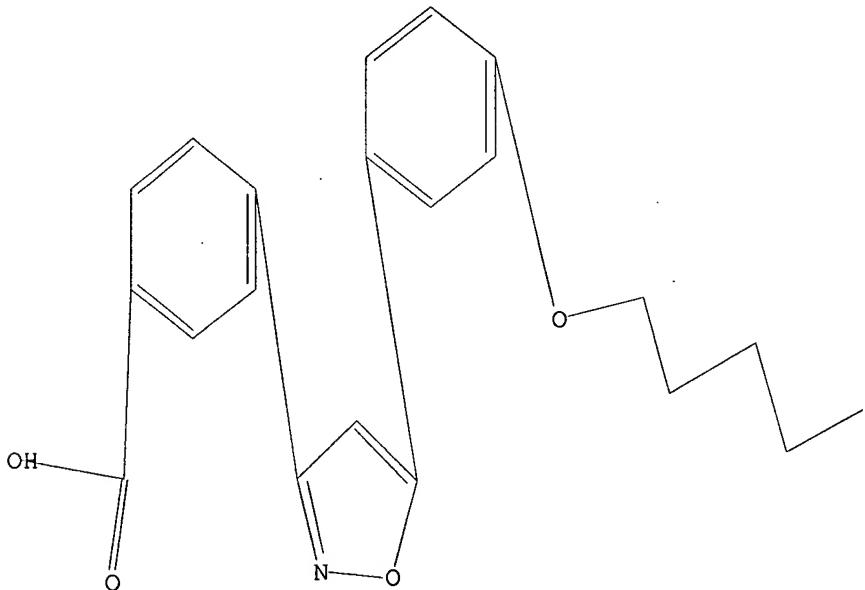
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS

L7 STRUCTURE UPLOADED

=> d

L7 HAS NO ANSWERS

L7 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 17 full

FULL SEARCH INITIATED 12:51:39 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 402 TO ITERATE

100.0% PROCESSED 402 ITERATIONS
SEARCH TIME: 00.00.01

7 ANSWERS

L8 7 SEA SSS FUL L7

=> file caplus
COST IN U.S. DOLLARS
FULL ESTIMATED COST

SINCE FILE ENTRY	TOTAL SESSION
166.94	527.95

FILE 'CAPLUS' ENTERED AT 12:51:43 ON 15 DEC 2006

10/522, 622 12/15/2006

10/522,622 12/15/2006

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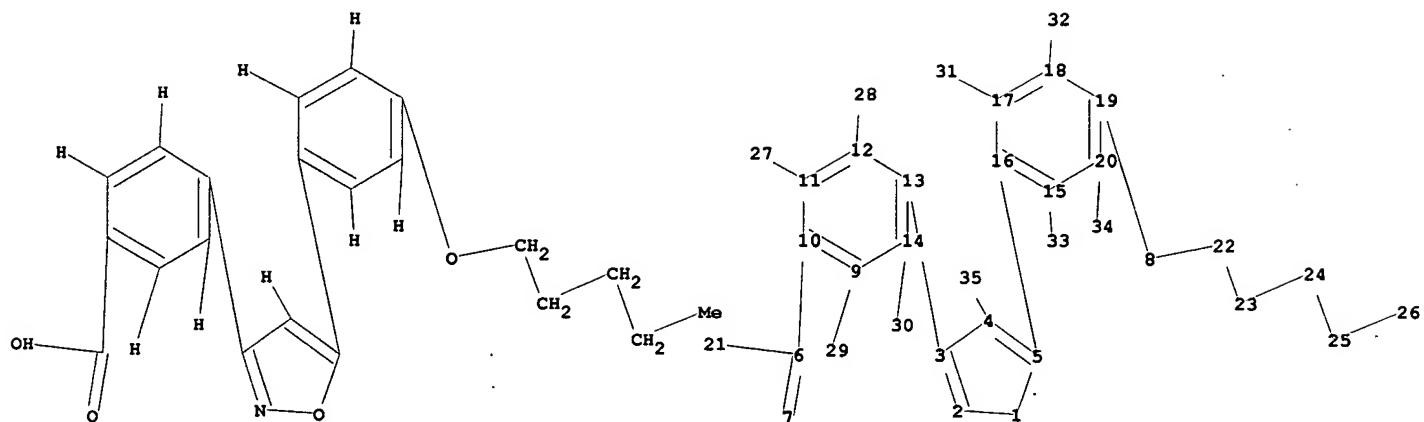
FILE COVERS 1907 - 15 Dec 2006 VOL 145 ISS 26
FILE LAST UPDATED: 14 Dec 2006 (20061214/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s 18
L9 5 L8
=> d ibib hitstr 1-5

10/522,622 12/15/2006



chain nodes :

6 7 8 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35

ring nodes :

1 2 3 4 5 9 10 11 12 13 14 15 16 17 18 19 20

chain bonds :

3-13 4-35 5-16 6-7 6-10 6-21 8-19 8-22 9-29 11-27 12-28 14-30 15-33 17-31
18-32 20-34 22-23 23-24 24-25 25-26

ring bonds :

1-2 1-5 2-3 3-4 4-5 9-10 9-14 10-11 11-12 12-13 13-14 15-16 15-20 16-17
17-18 18-19 19-20

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5 8-19

exact bonds :

3-13 4-35 5-16 6-10 8-22 9-29 11-27 12-28 14-30 15-33 17-31 18-32 20-34
22-23 23-24 24-25 25-26

normalized bonds :

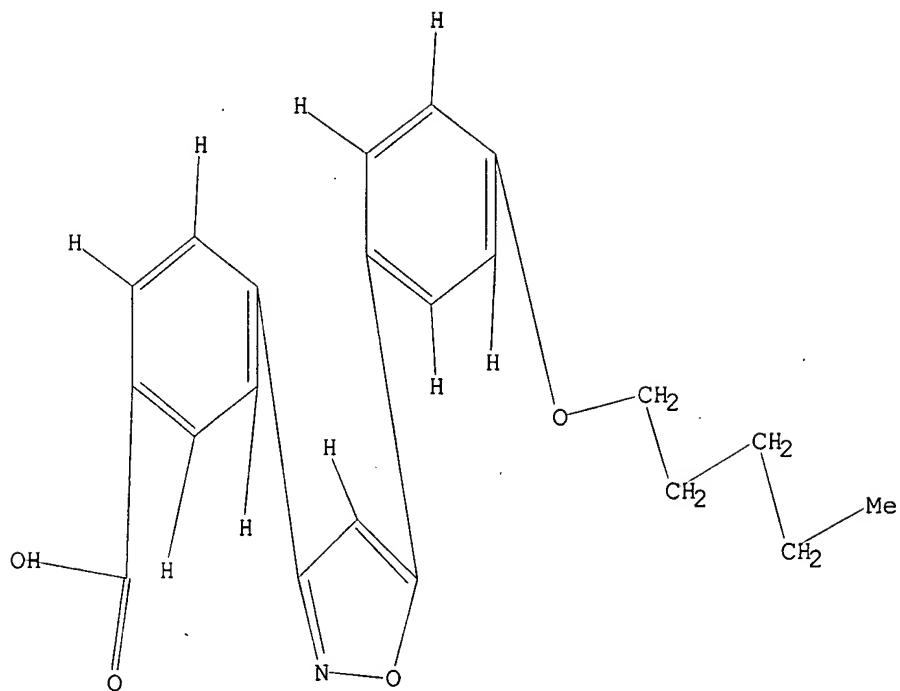
6-7 6-21 9-10 9-14 10-11 11-12 12-13 13-14 15-16 15-20 16-17 17-18 18-19
19-20

Match level :

 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:Atom 10:Atom
 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS
 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS

L1 STRUCTURE UPLOADED

 => d
 L1 HAS NO ANSWERS
 L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11 full
FULL SEARCH INITIATED 13:02:59 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 402 TO ITERATE

100.0% PROCESSED 402 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.01

L2 3 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS
SINCE FILE ENTRY TOTAL
SESSION
FULL ESTIMATED COST 166.94 167.15

FILE 'CAPLUS' ENTERED AT 13:03:03 ON 15 DEC 2006
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10/522,622 12/15/2006

FILE COVERS 1907 - 15 Dec 2006 VOL 145 ISS 26
FILE LAST UPDATED: 14 Dec 2006 (20061214/ED)

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=> s 12

L3 3 L2

=> d ibib hitstr 1-3

10/522,622 12/15/2006